Real-time reconstruction of arbitrary slices for quantitative and in-situ three-dimensional characterization of nanoparticles.

Introduction

Nanoparticles are important for a wide range of applications because of their unique properties, which are in general strongly connected to their 3D structure. To understand the connection between structure/composition and properties, nanoparticles are often investigated by transmission electron microscopy (TEM). Although TEM has become an indispensable tool to study nanomaterials, it remains difficult to perform a 3D characterization. Indeed, conventional TEM provides 2D projection images of 3D objects, therefore missing a wealth of information. Electron tomography was developed to overcome this issue.

During a typical electron tomography experiment, a series of 2D projection images are collected along a range of tilt angles, to cover an angular range that is as large as possible. After alignment of the tilt series, they serve as the input to a mathematical algorithm that reconstructs the 3D structure of the object. Both the alignment as the reconstruction of the acquired projection images are carried out through offline post-processing procedures, performed at a dedicated workstation.

These steps are computationally demanding, leading to a total data processing time of at least 1 hour. Since the alignment and reconstruction are performed offline, after the tilt series has been acquired, it is difficult or even impossible to identify potential problems concerning the acquisition parameters or the sample conditions during the TEM experiment. Consequently, efficient optimization of the experimental settings of a 3D in-situ experiment remains far from straightforward. The ability to extract information about the 3D structure of a nanoparticle during its TEM investigation would enable the operator to immediately perform additional, optimized or more detailed experiments for the same nanoparticle if necessary. In addition, to fully exploit the potential of in-situ holders and novel 3D acquisition methodologies, direct 3D visual feedback will be of essence to adjust the experimental parameters on-the-fly, in response to the observed dynamics of the nanoparticles. Clearly, realizing real-time 3D feedback would make a crucial impact in the field of 3D (in-situ) characterization of nanoparticles, which may even become as standard as conventional TEM.

Materials and methods

The electron tomography experiments were performed using a Thermo Fisher Scientific Tecnai Osiris operated at 200 kV. In-situ investigation was performed using the DENSsolutions tomography heating holder with MEMS-based heating chips. During the acquisition the open source RECAST3D software was used for visualization by real-time reconstruction.

Results

Here we present the open-source RECAST3D, to which novel computational components were added to enables real-time electron tomography. RECAST3D is based on the idea that inspecting a 3D reconstructed volume is typically carried out by slicing through the reconstructed volume in various suitable directions, effectively looking at a set of 2D slices. The software exploits the intrinsic speed of the FBP algorithm to reconstruct user-selected arbitrarily oriented 2D slices through the 3D structure in real time, without ever performing a full 3D volume reconstruction (**Figure 1**).

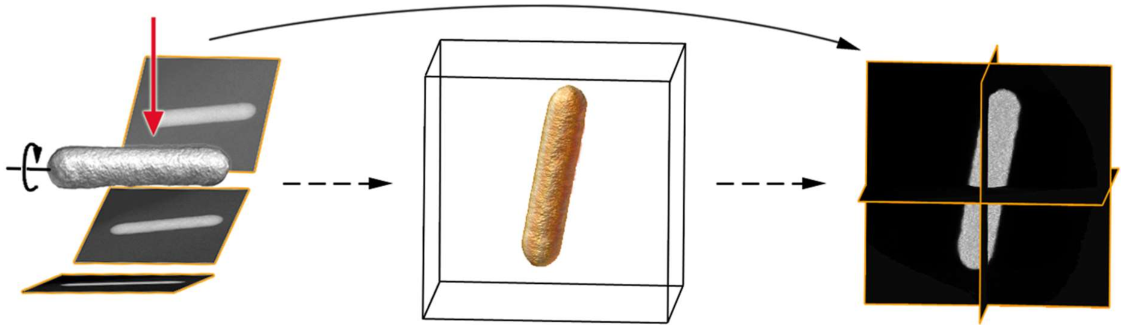

Figure 1: *Illustration of the workflow of a conventional tomography experiment (dashed arrows). First, 2D projection images are acquired. The direction of the electron beam is indicated by the red arrow. Next, a complete 3D reconstruction is performed. Finally, orthogonal 2D slices through the 3D reconstruction are investigated. RECAST3D provides a new approach (solid line) in which user selected slices are reconstructed on demand.*

Although such slices are 2D images, they represent subsets of the 3D inner structure of the sample under investigation. A combination of different slices therefore yields quasi-3D information. Moreover, these slices can be computed at any arbitrary position and along any angle, enabling the TEM operator to dynamically highlight features of interest of the investigated object. Since reconstructing 2D slices is computationally far less expensive and significantly more data efficient than reconstructing the entire 3D structure, slices can be automatically updated on-the-fly during the acquisition of a tilt series. Consequently, the quasi-3D tomographic view can be constructed in only a fraction of the time needed to acquire a regular 3D reconstruction of the entire structure, providing the groundwork for true real-time tomography. In addition to qualitative information, real-time quantitative information can be obtained as well. The RECAST3D software has support for user-written Python plugins, which can be used to perform real-time analysis of specific features in the reconstructed 2D slices. We showcase two different electron tomography studies during which RECAST3D was used beneficially, for steering the experimental (in-situ) parameters and improving the efficiency of the experiment.

Conclusion

We propose a new approach to compute high quality 2D slices through nanoparticles within approximately 60 ms, based on electron tomography tilt series. This technique is of great importance to improve the efficiency of 3D characterization of nanomaterials by TEM. It enables explorative imaging and provides valuable information to dynamically adjust the acquisition parameters during an electron tomography experiment. Moreover, quantification of specific features of nanoparticles becomes possible in real time, even while performing in-situ experiments.

References

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